FILE 'HOME' ENTERED AT 10:32:29 ON 23 DEC 2005

=> file registry
FILE 'REGISTRY' ENTERED AT 10:32:45 ON 23 DEC 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 22 DEC 2005   HIGHEST RN 870600-23-0
DICTIONARY FILE UPDATES: 22 DEC 2005   HIGHEST RN 870600-23-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

    Please note that search-term pricing does apply when
    conducting SmartSELECT searches.

****
*   *
* The CA roles and document type information have been removed from   *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005. A new display format, IDERL, is now   *
* available and contains the CA role and document type information.   *
*   *
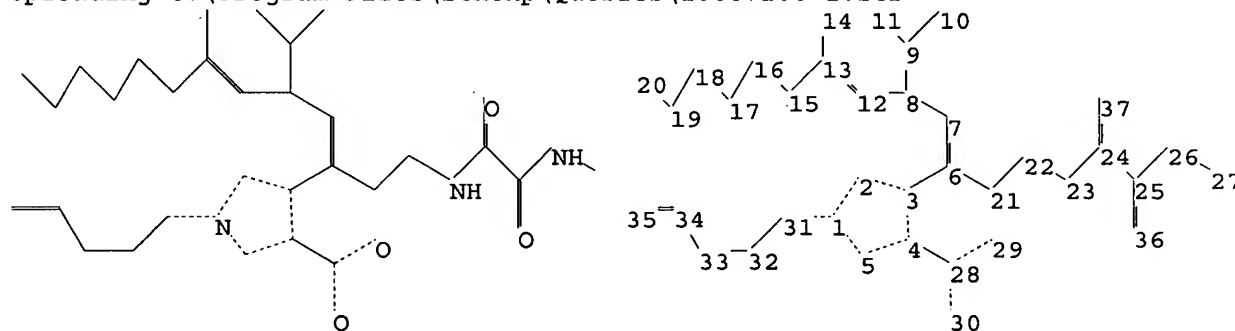***

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10667200-1.str

```
chain nodes :
6   7   8   9   10  11  12  13  14  15  16  17  18  19  20  21  22  23  24  25  26  27
28  29  30  31  32  33  34  35  36  37
ring nodes :
1   2   3   4   5
chain bonds :
1-31   3-6   4-28   6-7   6-21   7-8   8-9   8-12   9-10   9-11   12-13   13-14   13-15   15-16
16-17   17-18   18-19   19-20   21-22   22-23   23-24   24-25   24-37   25-26   25-36   26-27
28-29   28-30
31-32   32-33   33-34   34-35
ring bonds :
1-2   1-5   2-3   3-4   4-5
exact/norm bonds :
1-2   1-5   1-31   2-3   3-4   4-5   22-23   23-24   24-37   25-26   25-36   26-27   28-29
28-30

exact bonds :
3-6   4-28   6-7   6-21   7-8   8-9   8-12   9-10   9-11   12-13   13-14   13-15   15-16   16-17
17-18   18-19   19-20   21-22   24-25   31-32   32-33   33-34   34-35


Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:CLASS   7:CLASS   8:CLASS   9:CLASS   10:CLASS
11:CLASS   12:CLASS   13:CLASS   14:CLASS   15:CLASS   16:CLASS   17:CLASS   18:CLASS
19:CLASS   20:CLASS
21:CLASS   22:CLASS   23:CLASS   24:CLASS   25:CLASS   26:CLASS   27:CLASS   28:CLASS
29:CLASS   30:CLASS
31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS   36:CLASS   37:CLASS
```

L1   STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 10:33:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   0 TO ITERATE

100.0% PROCESSED   0 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE   **COMPLETE**
                          BATCH   **COMPLETE**
PROJECTED ITERATIONS: 0 TO   0
PROJECTED ANSWERS: 0 TO   0

L2   0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 10:33:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   2 TO ITERATE
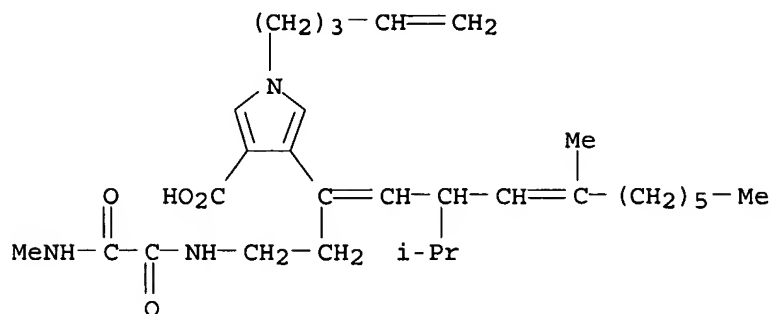
100.0% PROCESSED   2 ITERATIONS   1 ANSWERS
SEARCH TIME: 00.00.01

L3   1 SEA SSS FUL L1

=> d l3 ide

L3   ANSWER 1 OF 1   REGISTRY   COPYRIGHT 2005 ACS on STN
RN   674787-41-8   REGISTRY
ED   Entered STN: 13 Apr 2004
CN   1H-Pyrrole-3-carboxylic acid, 4-[5-methyl-1-[2-
      [[(methylamino)oxoacetyl]amino]ethyl]-3-(1-methylethyl)-1,4-undecadienyl]-

```
        1-(4-pentenyl)- (9CI)   (CA INDEX NAME)
FS    3D CONCORD
MF    C30 H47 N3 O4
SR    CA
LC    STN Files:   CA, CAPLUS, TOXCENTER, USPATFULL
```

$(CH_2)_3-CH\!=\!CH_2$ attached to N of a pyrrole ring; ring bears HO_2C and a side chain

$=CH-CH-CH\!=\!C-(CH_2)_5-Me$ with Me and $i\text{-}Pr$ substituents; $MeNH-C-C-NH-CH_2-CH_2$ with O carbonyls.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
          1 REFERENCES IN FILE CA (1907 TO DATE)
          1 REFERENCES IN FILE CAPLUS (1907 TO DATE)


=>

=>
Executing the logoff script...


=> LOG H
```

FILE & COST CENTER	QUANTITY @	RATE	ESTIMATED COST U.S. DOLLARS
REGISTRY FILE COST=			
CONNECT HOURS	0.04 @	37:00	1.48
INTERNET HOURS	0.04 @	6.00	0.24
DISPLAYS IN FORMAT IDE	1 @	1.84	1.84
ONL FUL SSS/CSS SEARCH TERMS	1 @	84.60	84.60
ONL FUL SSS/CSS SEARCHES	1 @	76.30	76.30

SUMMARY BY FILE AND	COST CENTER	HOURS	ESTIMATED COST U.S. DOLLARS
HOME FILE	(NONE)	0.01	0.21
REGISTRY FILE	(NONE)	0.04	164.46

COSTS INCLUDE TELECOMMUNICATION FEES		0.05	0.30

SUMMARY BY	COST CENTER	HOURS	ESTIMATED COST U.S. DOLLARS
	(NONE)	0.05	164.67
YOUR TOTAL SESSION COSTS ARE		0.05	164.67

```
  SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 10:35:09 ON 23 DEC 2005

Connecting via Winsock to STN
```

```
Welcome to STN International!  Enter x:x

LOGINID:SSSPTASXS1654

PASSWORD:
 * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 10:56:08 ON 23 DEC 2005
FILE 'REGISTRY' ENTERED AT 10:56:08 ON 23 DEC 2005
COPYRIGHT (C) 2005 American Chemical Society (ACS)

=> d his

      (FILE 'HOME' ENTERED AT 10:32:29 ON 23 DEC 2005)

      FILE 'REGISTRY' ENTERED AT 10:32:45 ON 23 DEC 2005
L1            STRUCTURE UPLOADED
L2         0 S L1
L3         1 S L1 FULL
L4            STRUCTURE UPLOADED
L5         0 S L4 FULL


=>
Uploading C:\Program Files\Stnexp\Queries\10667200-3.str
```
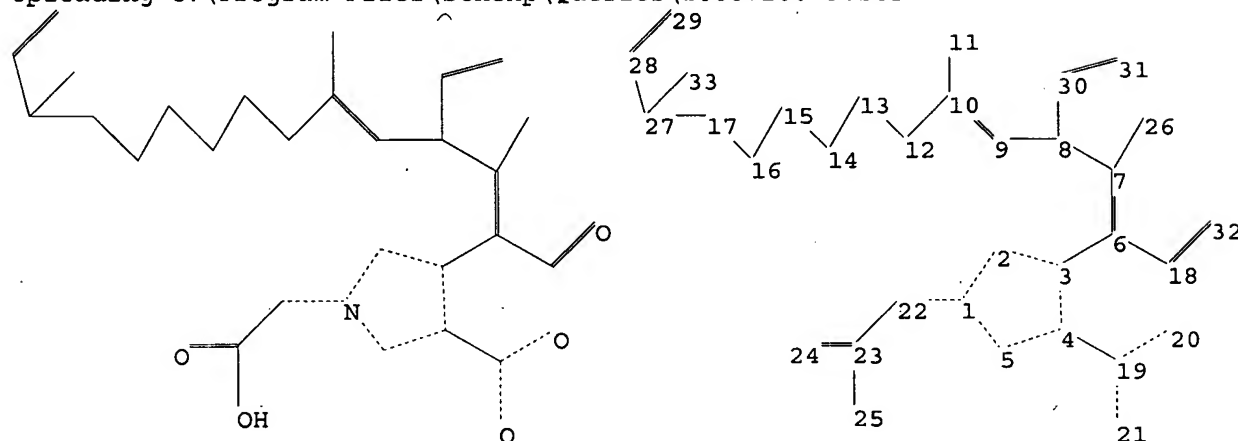


```
chain nodes :
6   7   8   9   10  11  12  13  14  15  16  17  18  19  20  21  22  23  24  25  26  27
28  29  30  31  32  33
ring nodes :
1   2   3   4   5
chain bonds :
1-22   3-6    4-19   6-7    6-18   7-8    7-26   8-9    8-30   9-10   10-11   10-12   12-13   13-14
14-15  15-16  16-17  17-27  18-32  19-20  19-21  22-23  23-24  23-25  27-28   27-33
28-29  30-31

ring bonds :
1-2   1-5   2-3   3-4   4-5
exact/norm bonds :
1-2   1-5   1-22   2-3   3-4   4-5   18-32   19-20   19-21
exact bonds :
3-6   4-19   6-7    6-18   7-8    7-26   8-9    8-30   9-10   10-11   10-12   12-13   13-14   14-15
```

```
15-16  16-17  17-27  22-23  27-28  27-33  28-29  30-31
normalized bonds :
23-24  23-25


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:CLASS  7:CLASS  8:CLASS  9:CLASS  10:CLASS
11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS  18:CLASS
19:CLASS  20:CLASS
21:CLASS  22:CLASS  23:CLASS  24:CLASS  25:CLASS  26:CLASS  27:CLASS  28:CLASS
29:CLASS  30:CLASS
31:CLASS  32:CLASS  33:CLASS




L6      STRUCTURE UPLOADED

=> s 16 full
FULL SEARCH INITIATED 10:56:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -        9 TO ITERATE

100.0% PROCESSED      9 ITERATIONS                        1 ANSWERS
SEARCH TIME: 00.00.01

L7              1 SEA SSS FUL L6

=>


=>
Executing the logoff script...


=> LOG H
```

FILE & COST CENTER	QUANTITY @	RATE	ESTIMATED COST U.S. DOLLARS
REGISTRY FILE COST=			
CONNECT HOURS	0.08 @	37.00	2.96
INTERNET HOURS	0.08 @	6.00	0.48
DISPLAYS IN FORMAT IDE	1 @	1.84	1.84
ONL FUL SSS/CSS SEARCH TERMS	3 @	84.60	253.80
ONL FUL SSS/CSS SEARCHES	3 @	76.30	228.90

SUMMARY BY FILE AND	COST CENTER	HOURS	ESTIMATED COST U.S. DOLLARS
HOME FILE	(NONE)	0.01	0.21
REGISTRY FILE	(NONE)	0.08	487.98

```
COSTS INCLUDE TELECOMMUNICATION FEES                 0.09        0.54
```

SUMMARY BY	COST CENTER	HOURS	ESTIMATED COST U.S. DOLLARS
	(NONE)	0.09	488.19
YOUR TOTAL SESSION COSTS ARE		0.09	488.19

```
  SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 10:57:11 ON 23 DEC 2005

Connecting via Winsock to STN
```
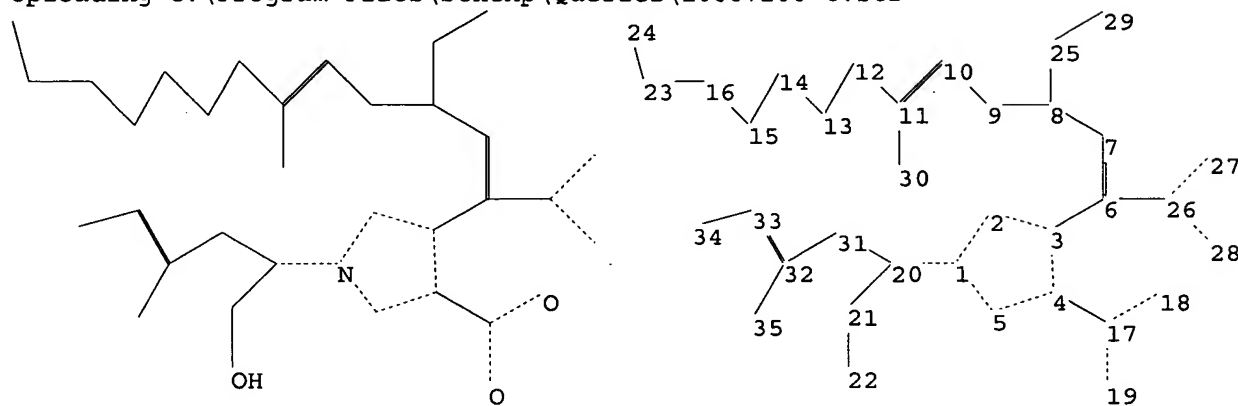
Welcome to STN International! Enter x:x

LOGINID:SSSPTASXS1654

PASSWORD:
 * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 11:03:24 ON 23 DEC 2005
FILE 'REGISTRY' ENTERED AT 11:03:24 ON 23 DEC 2005
COPYRIGHT (C) 2005 American Chemical Society (ACS)

=>
Uploading C:\Program Files\Stnexp\Queries\10667200-4.str

chain nodes :
6   7   8   9   10   11   12   13   14   15   16   17   18   19   20   21   22   23   24   25   26   27
28   29   30   31   32   33   34   35
ring nodes :
1   2   3   4   5
chain bonds :
1-20   3-6   4-17   6-7   6-26   7-8   8-9   8-25   9-10   10-11   11-12   11-30   12-13   13-14
14-15   15-16   16-23   17-18   17-19   20-21   20-31   21-22   23-24   25-29   26-27   26-28
31-32   32-33
32-35   33-34
ring bonds :
1-2   1-5   2-3   3-4   4-5
exact/norm bonds :
1-2   1-5   1-20   2-3   3-4   4-5   17-18   17-19   21-22   26-27   26-28
exact bonds :
3-6   4-17   6-7   6-26   7-8   8-9   8-25   9-10   10-11   11-12   11-30   12-13   13-14   14-15
15-16   16-23   20-21   20-31   23-24   25-29   31-32   32-33   32-35   33-34

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:CLASS   7:CLASS   8:CLASS   9:CLASS   10:CLASS
11:CLASS   12:CLASS   13:CLASS   14:CLASS   15:CLASS   16:CLASS   17:CLASS   18:CLASS
19:CLASS   20:CLASS
21:CLASS   22:CLASS   23:CLASS   24:CLASS   25:CLASS   26:CLASS   27:CLASS   28:CLASS
29:CLASS   30:CLASS
31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS

L8   STRUCTURE UPLOADED

=> s full l8
FULL SEARCH INITIATED 11:04:04 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   2 TO ITERATE

100.0% PROCESSED   2 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.01

L9   0 SEA SSS FUL L8

=> d his

     (FILE 'HOME' ENTERED AT 10:32:29 ON 23 DEC 2005)

     FILE 'REGISTRY' ENTERED AT 10:32:45 ON 23 DEC 2005
L1   STRUCTURE UPLOADED
L2   0 S L1
L3   1 S L1 FULL
L4   STRUCTURE UPLOADED
L5   0 S L4 FULL
L6   STRUCTURE UPLOADED
L7   1 S L6 FULL
L8   STRUCTURE UPLOADED
L9   0 S FULL L8

=> d ide 19
L9 HAS NO ANSWERS
'IDE ' IS NOT A VALID STRUCTURE FORMAT KEYWORD
Structure Formats
SIA ----- Structure Image, Attributes, and map table if it contains
          data. (Default)
SIM ----- Structure IMage.
SAT ----- Structure ATtributes and map table if it contains data.
SCT ----- Structure Connection Table and map table if it contains
          data.
SDA ----- All Structure DAta (image, attributes, connection table and
          map table if it contains data).
NOS ----- NO Structure data.
ENTER STRUCTURE FORMAT (SIM), NOS:end

=> d ide 17

L7   ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
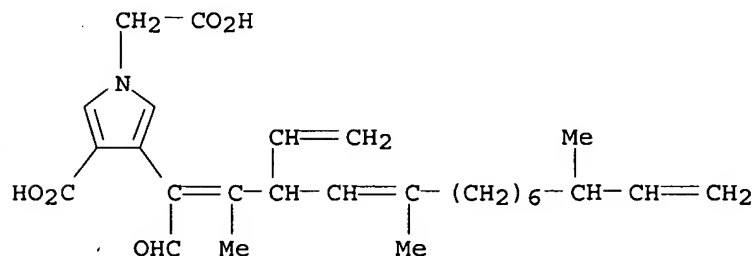RN   674787-44-1 REGISTRY
ED   Entered STN: 13 Apr 2004
CN   1H-Pyrrole-1-acetic acid, 3-carboxy-4-(3-ethenyl-1-formyl-2,5,12-trimethyl-
     1,4,13-tetradecatrienyl)- (9CI) (CA INDEX NAME)
FS   3D CONCORD
MF   C27 H37 N O5
SR   CA
LC   STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
                    1 REFERENCES IN FILE CA (1907 TO DATE)
                    1 REFERENCES IN FILE CAPLUS (1907 TO DATE)


=> file caplus
FILE 'CAPLUS' ENTERED AT 11:05:18 ON 23 DEC 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)
```

```
FILE COVERS 1907 - 23 Dec 2005   VOL 144 ISS 1
FILE LAST UPDATED: 22 Dec 2005   (20051222/ED)
```

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

```
=> s 13 17
MISSING OPERATOR L3 L7
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> s 13
L10            1 L3

=> s 17
L11            1 L7

=> d ibib abs hitstr l11 l10
L10 IS NOT VALID HERE
For an explanation, enter "HELP DISPLAY".

=> d ibib abs hitstr l11

L11  ANSWER 1 OF 1   CAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:      2004:252188   CAPLUS
DOCUMENT NUMBER:       140:266747
TITLE:                 Identification and modulation of substrate specificity
                       of secondary binding site of mammalian dipeptidyl
                       peptidase IV (DP IV) and applications in drug
                       screening and design
INVENTOR(S):           Hoffmann, Torsten; Kuehn-Wache, Kerstin; Demuth,
                       Hans-ulrich; Brandt, Wolfgang; Baer, Jochaim
PATENT ASSIGNEE(S):    Germany
SOURCE:                U.S. Pat. Appl. Publ., 51 pp.
                       CODEN: USXXCO
DOCUMENT TYPE:         Patent
LANGUAGE:              English
```

FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004058876	A1	20040325	US 2002-246817	20020918
WO 2004031374	A2	20040415	WO 2003-EP10408	20030918
WO 2004031374	A3	20040812		

```
        W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
            GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
            LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
            OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
            TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
       RW:  GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
            FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
            BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
   EP 1543023              A2    20050622     EP 2003-788909          20030918
        R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
```

PRIORITY APPLN. INFO.:   US 2002-246817   A 20020918
                                          US 2003-443417P   P 20030129
                                          WO 2003-EP10408   W 20030918

AB   The present application relates to the secondary binding site of mammalian
     dipeptidyl peptidase IV, its relationship amongst substrates and to the
     modulation of substrate specificity of dipeptidyl peptidase IV (DP IV,
     synonym: DPP IV, CD26, EC 3.4.14.5). The application provides compds.
     that bind to the secondary binding site of DP IV and their use to modulate
     the substrate specificity of DP IV; methods of treatment of various DP IV
     mediated disorders; and screening methods for the identification of
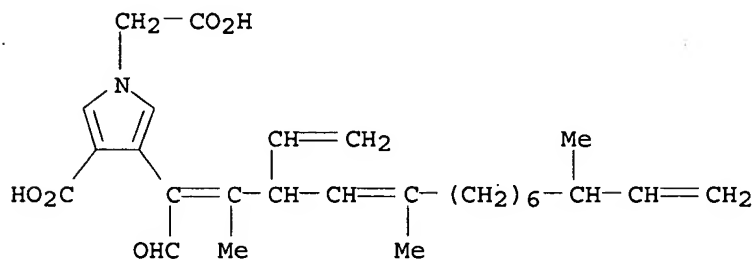   secondary binding sites on DP IV and DP IV-like enzymes.

IT   **674787-44-1**
     RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
       (identification and modulation of substrate specificity of secondary
       binding site of mammalian dipeptidyl peptidase IV (DP IV) and
       applications in drug screening and design)
RN   674787-44-1   CAPLUS
CN   1H-Pyrrole-1-acetic acid, 3-carboxy-4-(3-ethenyl-1-formyl-2,5,12-trimethyl-
     1,4,13-tetradecatrienyl)- (9CI)   (CA INDEX NAME)

$$CH_2-CO_2H$$

$$HO_2C \quad C=C-CH-CH=C-(CH_2)_6-CH-CH=CH_2$$

CH=CH₂ ... OHC   Me ... Me ... Me

```
=> d ibib abs hitstr l110
L110 NOT FOUND
The L-number entered has not been defined in this session, or it
has been deleted.  To see the L-numbers currently defined in this
session, enter DISPLAY HISTORY at an arrow prompt (=>).

=> d ibib abs hitstr 110
```

ACCESSION NUMBER: 2004:252188 CAPLUS
DOCUMENT NUMBER: 140:266747
TITLE: Identification and modulation of substrate specificity
                             of secondary binding site of mammalian dipeptidyl
                             peptidase IV (DP IV) and applications in drug
                             screening and design
INVENTOR(S):   Hoffmann, Torsten; Kuehn-Wache, Kerstin; Demuth,
                             Hans-ulrich; Brandt, Wolfgang; Baer, Jochaim
PATENT ASSIGNEE(S):   Germany
SOURCE: U.S. Pat. Appl. Publ., 51 pp.
                             CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004058876	A1	20040325	US 2002-246817	20020918
WO 2004031374	A2	20040415	WO 2003-EP10408	20030918
WO 2004031374	A3	20040812		

          W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
              CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
              GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
              LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
              OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
              TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
              KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
              FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
              BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

| EP 1543023 | A2 | 20050622 | EP 2003-788909 | 20030918 |

          R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

PRIORITY APPLN. INFO.:   US 2002-246817   A 20020918
                                           US 2003-443417P   P 20030129
                                           WO 2003-EP10408   W 20030918

AB   The present application relates to the secondary binding site of mammalian
     dipeptidyl peptidase IV, its relationship amongst substrates and to the
     modulation of substrate specificity of dipeptidyl peptidase IV (DP IV,
     synonym: DPP IV, CD26, EC 3.4.14.5). The application provides compds.
     that bind to the secondary binding site of DP IV and their use to modulate
     the substrate specificity of DP IV; methods of treatment of various DP IV
     mediated disorders; and screening methods for the identification of
     secondary binding sites on DP IV and DP IV-like enzymes.
IT   **674787-41-8**
     RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (identification and modulation of substrate specificity of secondary
         binding site of mammalian dipeptidyl peptidase IV (DP IV) and
         applications in drug screening and design)
RN   674787-41-8 CAPLUS
CN   1H-Pyrrole-3-carboxylic acid, 4-[5-methyl-1-[2-
     [[(methylamino)oxoacetyl]amino]ethyl]-3-(1-methylethyl)-1,4-undecadienyl]-
     1-(4-pentenyl)- (9CI)   (CA INDEX NAME)

$$(CH_2)_3-CH=CH_2$$

```
              (CH2)3 — CH = CH2
                      |
                      N
                     / \
                    ‖   \
                        ‖                         Me
                                                  |
         HO2C                   C = CH — CH — CH = C — (CH2)5 — Me
            \                  |            |
             (pyrrole)        |           i-Pr
                              |
   MeNH — C — C — NH — CH2 — CH2
         ‖   ‖
         O   O
```